PCR Example

This example shows how to compute Principal Component Regression (PCR) predictions. PCR can be computed with and without pre-processing. For PCR, pre-processing consists of mean-centering, which means to subtract out the mean from the data. This example shows how to compute PCR with and without mean-centering.

Supporting Information

A Practical Guide to Chemometric Analysis of Optical Spectroscopic Data

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PCR Algorithm

The PCR Algorithm is encapsulated in the following MATLAB function. If `meanCentered` is not entered, or if it is false, then pre-processing (mean centering) is not done. If `meanCentered` is true, then pre-processiing (mean centering) is done.

```
function [C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents,
meanCentered)
    %pnnl_pcr Principal component regression (PCR)
    %
    %   [C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents) returns
    %   concentration matrix C_pcr based on the first nPrincipalComponents principal
    %   components of the singular values of A_train.  Multiplier
    %   matrix B_pcr is the pseudo-inverse of Beer's law extinction
    %   coefficient matrix such that C_pcr = A_unknown * B_pcr.
    %
    %   pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents, meanCentered) applies mean
    %   centering when meanCentered is true, and does not apply mean
    %   centering when meanCentered is false.  When meanCentered is not
    %   supplied, the default is false (no mean centering).
    %
    %   Example:
```

```
    %
    %     load pnnl_napalm_data
    %     nPrincipalComponents = 3;
    %     [C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents);
    %
    %   See also pnnl_cls, pnnl_pls.

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    if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end

    [U,S,V] = svd(X0,'econ');
    B_pcr = V(:,1:nPrincipalComponents) / S(1:nPrincipalComponents,1:nPrincipalComponents) *
U(:,1:nPrincipalComponents)' * Y0;

    if meanCentered
        C_pcr = (A_unknown - mean(A_train,1)) * B_pcr + mean(C_train,1);
    else
        C_pcr = A_unknown * B_pcr;
    end
end
```

Concentration Data

The concentrations of the training data are in matrix `C_train` and the concentrations of the validation data are in matrix `C_validation`. Column 1 corresponds to the concentrations in constituent 1 (benzene). Column 2 corresponds to the concentrations in constituent 2 (polystyrene). Column 3 corresponds to the concentrations in constituent 3 (gasoline).

$$C_{\text{train}} = \begin{array}{rrrr} \textit{benzene} & \textit{polystyrene} & \textit{gasoline} & \\ 0 & 0 & 100.0000 & 1 \\ 5.1309 & 0 & 94.8691 & 2 \\ 10.0660 & 0 & 89.9300 & 3 \\ 20.1799 & 0 & 79.8201 & 4 \\ 40.0120 & 0 & 59.9878 & 5 \\ 59.9972 & 0 & 40.0028 & 6 \\ 79.8412 & 0 & 20.1588 & 7 \\ 89.8273 & 0 & 10.1727 & 8 \\ 100.0000 & 0 & 0 & 9 \\ 90.0264 & 9.9736 & 0 & 10 \\ 80.1375 & 19.8625 & 0 & 11 \\ 64.9950 & 35.0005 & 0 & 12 \\ 21.0228 & 45.9197 & 33.0575 & 13 \\ 49.9507 & 5.0599 & 44.9895 & 14 \\ 40.0182 & 20.0385 & 39.9433 & 15 \\ 40.0154 & 10.0036 & 49.9810 & 16 \\ 30.0059 & 10.0282 & 59.9659 & 17 \\ 40.0340 & 39.9670 & 19.9990 & 18 \\ 49.9393 & 3.3748 & 46.6859 & 19 \\ 46.6501 & 13.4658 & 39.8840 & 20 \end{array}$$

$$C_{\text{validation}} = \begin{array}{rrrr} \textit{benzene} & \textit{polystyrene} & \textit{gasoline} & \\ 22.1665 & 39.0384 & 38.7951 & 1 \\ 21.6874 & 37.0596 & 41.2530 & 2 \\ 22.1665 & 39.6980 & 38.1355 & 3 \\ 26.9575 & 40.3576 & 32.6849 & 4 \\ 25.9993 & 33.7616 & 40.2391 & 5 \\ 23.1247 & 37.0596 & 39.8157 & 6 \\ 22.6456 & 39.0384 & 38.3160 & 7 \\ 22.6456 & 39.0384 & 38.3160 & 8 \\ 27.4366 & 42.3364 & 30.2270 & 9 \\ 27.4366 & 37.7192 & 34.8442 & 10 \\ 26.4784 & 40.3576 & 33.1640 & 11 \\ 26.9575 & 37.7192 & 35.3233 & 12 \end{array}$$

Clear variables and load the PNNL napalm data.

```
clearvars
load pnnl_napalm_data
```

PCR with and without pre-processing

Choose the number of principal components.

```
nPrincipalComponents = 3;
```

Set meanCentered to true to indicate that pre-processing (mean centering) is done, and false to indicate that pre-processing (mean centering) is not done.

```
for meanCentered = [true, false]
```

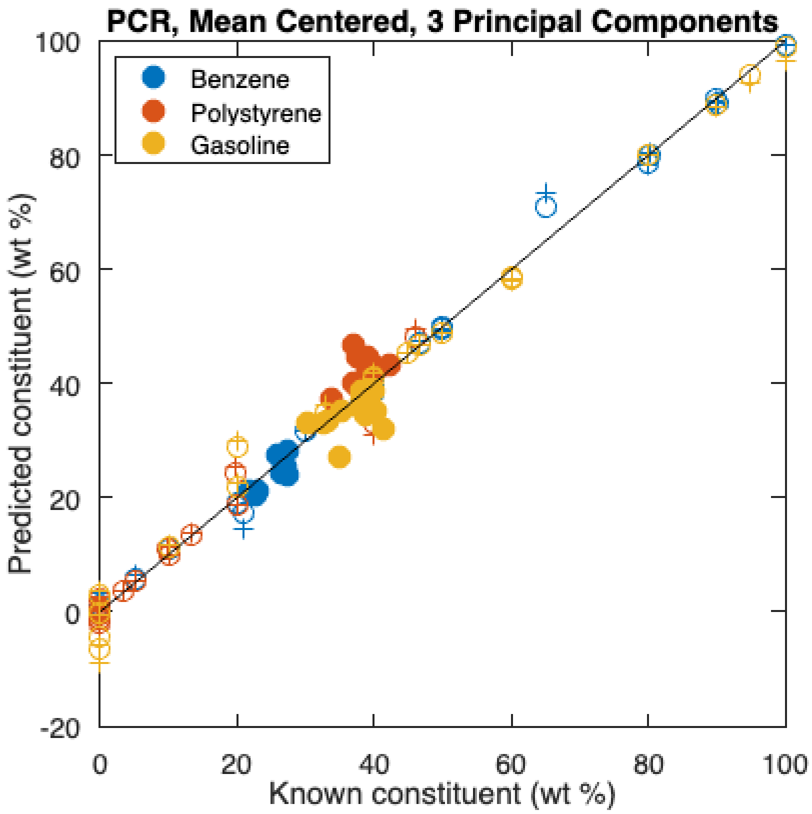
Set up the plot title and color.

```
    LogicalStr = {'Not ',''};
    title_string = sprintf('PCR, %sMean Centered, %d Principal 
Components',LogicalStr{meanCentered+1},nPrincipalComponents);
    nConstituents = size(C_validation,2);
    colorOrder = pnnl_colorOrder(nConstituents);
```

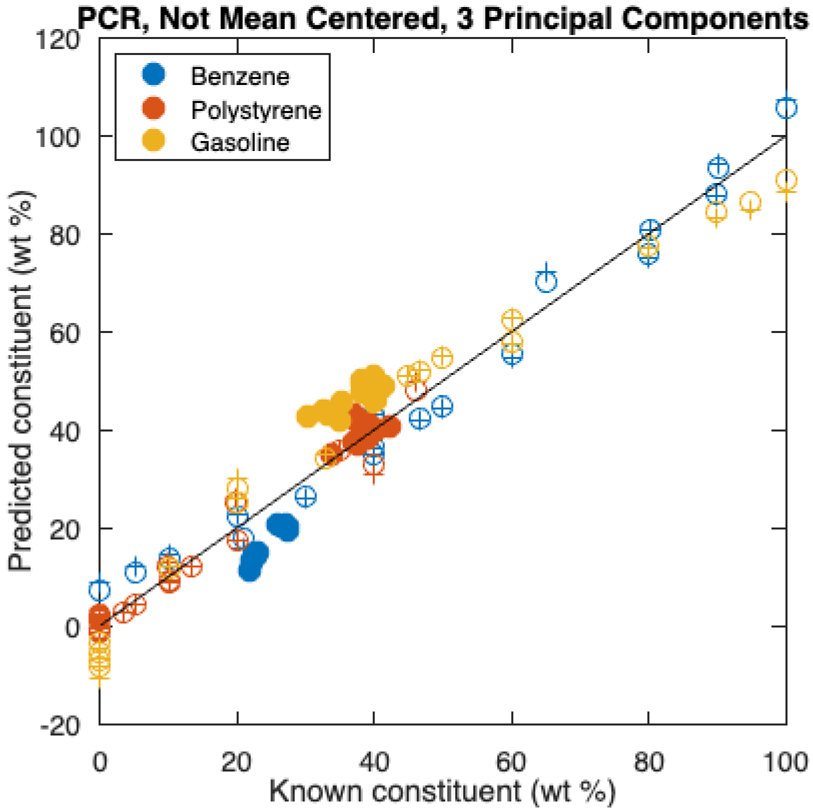
Use the columns of `C_train` to compute PCR. Use the columns of `C_validation` to compute RMSEP (root mean square error predicted). Use the columns of `C_train` to compute RMSEC (root mean square error calibration) and RMSECV (root mean square error cross validation).

```
    % Compute PCR
    C_predicted =
pnnl_pcr(A_train,C_train,A_unknown,nPrincipalComponents,meanCentered);
    C_calibration =
pnnl_pcr(A_train,C_train,A_train,nPrincipalComponents,meanCentered);
    C_cross_validation =
pnnl_cross_validation(@pnnl_pcr,A_train,C_train,nPrincipalComponents,meanCen
tered);
    % Compute RMSE
    RMSEP = pnnl_rmse(C_validation,C_predicted);
    RMSEC = pnnl_rmse(C_train,C_calibration);
    RMSECV = pnnl_rmse(C_train,C_cross_validation);
    % Display RMSE
    pnnl_display_rmse(title_string,ConstituentNames,RMSEC,RMSECV,RMSEP);

    % Plot results
    figure
    h = gobjects(nConstituents,1);
    for k = 1:nConstituents
        % Plot Concentrations
        hold on
        % Validation vs. Predicted
        h(k) =
plot(C_validation(:,k),C_predicted(:,k),'.','MarkerSize',35,'Color',colorOrd
er(k,:),'DisplayName',ConstituentNames{k});
        % Train vs. Calibration

plot(C_train(:,k),C_calibration(:,k),'o','MarkerSize',10,'LineWidth',1,'Colo
r',colorOrder(k,:))
        % Train vs. Crosss Validation

plot(C_train(:,k),C_cross_validation(:,k),'+','MarkerSize',10,'LineWidth',1,
'Color',colorOrder(k,:))
        % 1-1 line
        line(C_train(:,k),C_train(:,k),'Color','k')
        title(title_string)
        xlabel(['Known constituent (',ConcentrationUnits,')'])
        ylabel(['Predicted constituent (',ConcentrationUnits,')'])
        set(gca,'FontSize',14)
        box on
        axis square
        hold off
    end
    legend(h,'Location','northwest')
    disp('Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.')
end
```

```
-------------------------------------------------------------------------------------
  PCR, Mean Centered, 3 Principal Components       Benzene   Polystyrene      Gasoline
                                       RMSEC        1.8648        2.0907        2.8637
                                      RMSECV        2.7229        2.7118         3.677
                                       RMSEP        1.9451        4.4554        4.1347
-------------------------------------------------------------------------------------
```



```
Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.
-----------------------------------------------------------------------------------------
  PCR, Not Mean Centered, 3 Principal Components       Benzene   Polystyrene      Gasoline
                                           RMSEC        4.2787        2.3856        5.6681
                                          RMSECV        5.1022        2.9924        6.7526
                                           RMSEP        7.7847        2.2831        9.9695
-----------------------------------------------------------------------------------------
```



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

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